

# $^4\text{He}$ energies and radii by the coupled-cluster method with many-body average potential

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The reformulated coupled-cluster method (CCM), in which average many-body potentials are introduced, provides a useful framework to organize numerous terms appearing in CCM equations, which enables us to clarify the structure of the CCM theory and physical importance of various terms more easily. We explicitly apply this framework to  $^4\text{He}$ , retaining one-body and two-body correlations as the first illustrating attempt. Numerical results with using two modern nucleon-nucleon interactions (AV18 and CD-Bonn) and their low-momentum interactions are presented. The characters of short-range and many-body correlations are discussed. Although not considered explicitly, the expression of the ground-state energy in the presence of a three-nucleon force is given.

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## I. INTRODUCTION

The understanding of various properties of atomic nuclei starting from the realistic nucleon-nucleon interactions is one of fundamental problems in the theoretical nuclear physics. The recent studies in this field are characterized by several new developments. Resulting from developments through 1960's and 1990's, there are now various parameterizations of the nucleon-nucleon interaction which reproduce experimental two-body scattering and deuteron data with high precision. Systematic introduction of a three-nucleon force is in progress especially in the framework of the new development of the potential description in the chiral effective field theory [1, 2]. Progress is also seen in an effective interaction theory in a restricted space, driven by active studies of low-momentum interactions [3]. In addition, various ab-initio frameworks of many-body calculations have been explicitly applied to atomic nuclei, such as a Monte-Carlo method [4], a no-core shell model [5] and a coupled-cluster method (CCM) [6]. Among them, the CCM is a promising method toward heavier nuclei because of the advantage of the size-extensivity.

The CCM was devised for many-body problems in nuclear physics in 1950's [7, 8] and the achievements in 1970's by the Bochum group were reported in Ref. [9]. It was, however, almost discarded in nuclear physics community. The CCM found its place in quantum chemistry [10, 11] as a tool of the first-principle calculation. The method was reintroduced around 2000 in the description of atomic nuclei [6, 12]. Because there are specific difficulties in a description and a treatment of the short-range part of a nucleon-nucleon interaction, applications of the CCM to nuclei require deeper understanding of an

effective interaction theory. It is not surprising that a renewed interest arises in the CCM in parallel with the development of low-momentum interaction theory [3].

There is already a considerable number of CCM calculations of light nuclei in recent years [6, 13–17]. These include the extension to excited states [13, 17], nuclei far from the stability line [15] and heavier nuclei such as  $^{40,48}\text{Ca}$  [14, 16]. Contributions of a three-nucleon force has also been estimated in this method [18]. Nevertheless, because of the usefulness of the CCM framework to solve the quantum many-body problem as exactly as possible, it is important to clarify the structure of this framework as much as possible and to try to obtain the physical understanding of various correlations in a transparent way. Such an attempt was proposed by Suzuki [19] in the early 1990's as an application of the similarity-transformation theory for a quantum-mechanical eigenvalue problem. His reformulation introduces average many-body potentials as the generalization of the one-body mean field. The concept of the mean field is essentially important in almost all many-body systems, as the independent single-particle model is empirically established in those systems. As is shown below, the many-body average field is useful to group various terms which appear in the CCM practical calculations, and thus is helpful to elucidate the structure of the CCM many-body correlations. The transformation of the Hamiltonian to the normal ordered form with respect to the reference state is inherent in this formulation. Unfortunately, explicit applications of this method to nuclei has not been carried out so far. It is useful at the present stage to promote this formulation for the description of actual nuclei with using the realistic nucleon-nucleon interaction, in view of the future wide use of the CCM framework in nuclear many-body problems.

We recapitulate the CCM formulation with introducing average many-body potentials in Sec. II, starting with the basic idea of the CCM. Although we do not

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consider the contribution of a three-nucleon force in the present numerical calculations, the expression including three-body terms are presented in the initial part of Sec. II. As the first attempt of the actual application of this method to nuclei, we employ the approximation in which only one-body and two-body amplitudes are retained. This truncation is referred to as CCSD in the literature. Numerical calculations are carried out for  ${}^4\text{He}$  with using two modern nucleon-nucleon potentials, the CD-Bonn potential [20] and the Argonne AV18 potential [21]. Results of the energy and radius of  ${}^4\text{He}$  in a harmonic oscillator model space are presented in Sec. III. First, results with the bare potentials are shown, and then the calculations with low-momentum equivalent interactions are discussed. The magnitude of the contributions from the average many-body potential is estimated. The independence of the results on the harmonic oscillator constant of the reference state is demonstrated. If we do not include one-body amplitudes, the results varies with changing the oscillator constant. Conclusions follow in Sec. IV.

## II. COUPLED-CLUSTER METHOD

We first give the idea of the CCM in its naive form, and next present the introduction of many-body average potentials.

### A. Basic

The basic ansatz of the coupled-cluster method [7, 8] is that the exact state  $|\Psi\rangle$  of the Hamiltonian  $H$  of  $A$  particles with the mass  $m$  is given by the transformation operator  $e^S$  acting on the reference state  $|\Phi_0\rangle$ :

$$|\Psi\rangle = e^S |\Phi_0\rangle. \quad (1)$$

The Hamiltonian  $H$  consists of the one-body kinetic energy  $t_i = \frac{\hbar^2}{2m} \mathbf{k}_i^2$ , the two-nucleon interaction  $v_{ij}$ , the three-nucleon interaction  $v_{ijk}$ , and so on. To be explicit, we write the Hamiltonian as follows.

$$H = \sum_i \frac{\hbar^2}{2m} \mathbf{k}_i^2 - T_G + \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk}, \quad (2)$$

where  $T_G$  denotes the center-of-mass kinetic operator. In the following, we absorb the one-body part of  $T_G$  in the one-body kinetic energy, namely the operator being  $t_i = \frac{A-1}{A} \frac{\hbar^2}{2m} \mathbf{k}_i^2$ , and the two-body part of  $T_G$  in the two-body interaction  $v_{ij}$ .

Solving the time-independent Schrödinger equation

$$H e^S |\Phi_0\rangle = E_0 e^S |\Phi_0\rangle, \quad (3)$$

is to determine the transformation operator  $S$ , which consists of one-body part, two-body part, and up to  $A$ -body part.

$$S = \sum_i s_i + \sum_{i<j} s_{ij} + \sum_{i<j<k} s_{ijk} + \cdots + s_{12\cdots A}. \quad (4)$$

We refer to single-particle states in  $|\Phi_0\rangle$  as hole states denoted by  $h$  and other single-particle states as particle states denoted by  $p$ . By definition, only the particle (hole) states appear in the bra (ket) configuration of the transformation amplitude  $\langle p_1 p_2 \cdots p_n | s_{12\cdots n} | h_1 h_2 \cdots h_n \rangle_A$ , where the suffix  $A$  means an antisymmetrized matrix element; namely,  $|h_1 h_2\rangle_A \equiv |h_1 h_2 - h_2 h_1\rangle$ ,  $|hh'h''\rangle_A \equiv |hh'h'' - hh''h' + h'h''h - h'hh'' + h''hh' - h''h'h\rangle$  and so on.

The prescription of the CCM is to rewrite the Schrödinger equation (3) as

$$e^{-S} H e^S |\Phi_0\rangle = E_0 |\Phi_0\rangle. \quad (5)$$

It is noted that in the standard CCM theory, the Hamiltonian is supposed to be normal-ordered with respect to the reference state at this stage. Hence we denote the Hamiltonian by  $H_n$ . The operator  $S$  is determined by the decoupling equation for the similarity-transformed Hamiltonian  $e^{-S} H_n e^S$ :

$$\langle np - nh | e^{-S} H_n e^S | \Phi_0 \rangle = 0, \quad (6)$$

with  $n = 1, 2, \cdots A$ . Here,  $\langle np - nh |$  represents an arbitrary  $n$ -particle and  $n$ -hole state. Determining  $S$ , the energy is given by

$$E_0 = \langle \Phi_0 | e^{-S} H_n e^S | \Phi_0 \rangle. \quad (7)$$

The similarity-transformation  $e^{-S} H_n e^S$  may be evaluated systematically by the Baker-Campbell-Hausdorff formula:

$$e^{-S} H_n e^S = H_n + [H_n, S] + \frac{1}{2!} [[H_n, S], S] + \cdots \quad (8)$$

In practice, the Hamiltonian should be rearranged in the normal-order form with respect to  $|\Phi_0\rangle$  [6, 22]. The transparent procedure of the transformation in view of the effective interaction theory was formulated by Suzuki [19]. This method with introducing many-body average potentials is outlined in the next subsection.

### B. Many-body average potential

When the original Hamiltonian  $H$  do not have more than three-nucleon interactions, the expansion of  $e^{-S} H e^S$  terminates with the four-folded commutator and produces various terms up to six-body operators. If a three-nucleon interaction is present, more than five-folded commutators appear. Suzuki and collaborators [19, 23] reformulated the CCM by introducing many-body average fields, which enables us to write down the decoupling equations in a compact form and thus to clarify the structure of various many-body correlations. We manipulate explicit expressions in this formulation and carry out numerical calculations.

The similarity-transformed Hamiltonian may be reorganized by introducing an auxiliary many-body potential

$$U = \sum_i u_i + \sum_{i<j} u_{ij} + \sum_{i<j<k} u_{ijk} + \cdots \quad (9)$$

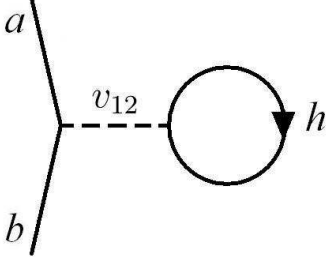


FIG. 1: Bubble insertion diagram for Hartree-Fock mean field. The antisymmetrization is not shown explicitly.

$$\begin{aligned}
 &= \sum_i (\tilde{h}_i - \tilde{u}_i) + \sum_{i < j} (\tilde{v}_{ij} - \tilde{u}_{ij}) \\
 &\quad + \sum_{i < j < k} (\tilde{v}_{ijk} - \tilde{u}_{ijk}) + \dots
 \end{aligned} \tag{11}$$

The prototype of the auxiliary potential for a many-body system is a Hartree-Fock one. The one-body Hartree-Fock mean field for states  $|a\rangle$  and  $|b\rangle$  is defined by folding two-body interactions with respect to occupied states  $|h\rangle$ :

The transformed Hamiltonian is written as

$$\begin{aligned}
 e^{-S} H e^S &= e^{-S} (H + U) e^S - e^{-S} U e^S \\
 &= \left\{ \sum_i \tilde{h}_i + \sum_{i < j} \tilde{v}_{ij} + \sum_{i < j < k} \tilde{v}_{ijk} + \dots \right\} \\
 &\quad - \left\{ \sum_i \tilde{u}_i + \sum_{i < j} \tilde{u}_{ij} + \sum_{i < j < k} \tilde{u}_{ijk} + \dots \right\}
 \end{aligned} \tag{10}$$

That is,

$$e^{-S} \left\{ \sum_i t_i + \sum_{i < j} v_{ij} + \sum_{i < j < k} v_{ijk} \right\} e^S$$

$$\langle a | u_{HF} | b \rangle = \sum_h \langle a h | v_{12} | b h \rangle_A. \tag{12}$$

The summation is depicted as a bubble insertion diagram of Fig. 1. The formulation by Suzuki *et al.* [19, 23] generalize the HF potential to many-body states. That is, the auxiliary potential  $U$  is determined so as to cancel all the bubble-insertion contributions.

$$\langle a_1 \dots a_n | \tilde{u}_{1\dots n} | b_1 \dots b_n \rangle_A = \sum_{k \geq 1} \frac{(-1)^{k+1}}{k!} \sum_{h_1 \dots h_k} \langle a_1 \dots a_n h_1 \dots h_k | \tilde{v}_{1\dots n+k} | b_1 \dots b_n h_1 \dots h_k \rangle_A, \tag{13}$$

where  $a$  and  $b$  stand for either particle or hole state. It is instructive to give explicit expressions for the one-body  $\tilde{u}_1$  and the two-body  $\tilde{u}_{12}$ .

$$\langle a | \tilde{u}_1 | b \rangle = \sum_h \langle a h | \tilde{v}_{12} | b h \rangle_A - \frac{1}{2!} \sum_{hh'} \langle a h h' | \tilde{v}_{123} | b h h' \rangle_A + \frac{1}{3!} \sum_{hh'} \langle a_1 a_2 h h' | \tilde{v}_{1234} | b_1 b_2 h h' \rangle_A + \dots, \tag{14}$$

$$\langle a_1 a_2 | \tilde{u}_{12} | b_1 b_2 \rangle_A = \sum_h \langle a_1 a_2 h | \tilde{v}_{123} | b_1 b_2 h \rangle_A - \frac{1}{2!} \sum_{hh'} \langle a_1 a_2 h h' | \tilde{v}_{1234} | b_1 b_2 h h' \rangle_A + \dots \tag{15}$$

It is apparent that  $\tilde{u}$  is a sum of bubble-insertion contributions of the similarity-transformed interactions, if we rewrite the above definition of  $\tilde{u}_1$  as

$$\begin{aligned}
 \langle a | \tilde{u}_1 | b \rangle &= \sum_h \langle a h | \tilde{v}_{12} - \tilde{u}_{12} | b h \rangle_A + \sum_h \langle a h | \tilde{u}_{12} | b h \rangle_A - \frac{1}{2!} \sum_{hh'} \langle a h h' | \tilde{v}_{123} | b h h' \rangle_A \\
 &\quad + \frac{1}{3!} \sum_{hh'h''} \langle a h h' h'' | \tilde{v}_{1234} | b h h' h'' \rangle_A + \dots,
 \end{aligned} \tag{16}$$

$$\begin{aligned}
 &= \sum_h \langle a h | \tilde{v}_{12} - \tilde{u}_{12} | b h \rangle_A + \frac{1}{2!} \sum_{hh'} \langle a h h' | \tilde{v}_{123} | b h h' \rangle_A + \left( \frac{1}{3!} - \frac{1}{2!} \right) \sum_{hh'h''} \langle a h h' h'' | \tilde{v}_{1234} | b h h' h'' \rangle_A + \dots \\
 &= \sum_h \langle a h | \tilde{v}_{12} - \tilde{u}_{12} | b h \rangle_A + \frac{1}{2!} \sum_{hh'} \langle a h h' | \tilde{v}_{123} - \tilde{u}_{123} | b h h' \rangle_A + \frac{1}{3!} \sum_{hh'h''} \langle a h h' h'' | \tilde{v}_{1234} | b h h' h'' \rangle_A + \dots,
 \end{aligned} \tag{17}$$

and also for  $\tilde{u}_{12}$

$$\langle a_1 a_2 | \tilde{u}_{12} | b_1 b_2 \rangle_A = \sum_h \{ \langle a_1 a_2 h | \tilde{v}_{123} - \tilde{u}_{123} | b_1 b_2 h \rangle_A + \langle a_1 a_2 h | \tilde{u}_{123} | b_1 b_2 h \rangle_A \} - \frac{1}{2!} \sum_{hh'} \langle a_1 a_2 h h' | \tilde{v}_{1234} | b_1 b_2 h h' \rangle_A + \dots$$

$$= \sum_h \langle a_1 a_2 h | \tilde{v}_{123} - \tilde{u}_{123} | b_1 b_2 h \rangle_A + \frac{1}{2!} \sum_{hh'} \langle a_1 a_2 h h' | \tilde{v}_{1234} | b_1 b_2 h h' \rangle_A + \dots \quad (18)$$

Therefore,  $e^{-S}(H+U)e^S$  is now arranged in the normal-ordered form with respect to the reference state. It means that the following decoupling conditions should be imposed.

$$\langle np - nh | e^{-S}(H+U)e^S | \Phi_0 \rangle = 0. \quad (19)$$

This corresponds to considering the decoupling condition for the normal-ordered Hamiltonian  $H_n$  in the standard CCM, Eq. (6). The potential  $U$  thus defined may be called a many-body average potential.

To proceed to actual calculations, explicit expressions of the similarity-transformed interaction  $e^{-S}He^S$  are needed. The result of the straightforward calculation is given in the Appendix. In these expressions the terms including a three-nucleon interaction and a three-body amplitude  $s_{ijk}$  are retained. However, because we do not consider these contributions in the CCSD truncation in this paper, we do not keep these terms here after.

### C. Decoupling equations and energy

Some manipulation is necessary to obtain explicit expressions of matrix elements of  $\tilde{u}$  in terms of the original

interactions  $v_{12}$  and the correlation amplitudes  $s_1$  and  $s_{12}$ . Because  $\tilde{h}_1 = e^{-s_1}t_1e^{s_1} + \tilde{u}_1 = (1-s_1)t_1(1+s_1) + \tilde{u}_1$ , the one-particle-one-hole decoupling equation becomes

$$\langle p | \tilde{h}_1 | h \rangle = \langle p | (1-s_1)t_1(1+s_1) + \tilde{u}_1 | h \rangle = 0. \quad (20)$$

The explicit expression of  $\langle p | \tilde{u}_1 | h \rangle$  is given below, Eq. (27). Next, the two-particle-two-hole decoupling equation  $\langle p_1 p_2 | \tilde{v}_{12} | h_1 h_2 \rangle_A = 0$  reads

$$\begin{aligned} & \langle p_1 p_2 | \tilde{v}_{12} - \tilde{u}_{12} + \tilde{u}_{12} | h_1 h_2 \rangle_A \\ &= \langle p_1 p_2 | (1-s_1-s_2+s_1s_2-s_{12})v_{12} \\ & \times (1+s_1+s_2+s_1s_2+s_{12}) + \tilde{u}_{12} | h_1 h_2 \rangle_A = 0. \end{aligned} \quad (21)$$

Figuring out the explicit form of the matrix element  $\langle p_1 p_2 | \tilde{u}_{12} | h_1 h_2 \rangle_A$  according to Eq. (18), this equation can be written in the following rather compact manner:

$$\begin{aligned} & \langle p_1 p_2 | (1-s_1-s_2+s_1s_2+s_{12})v_{12}(1+s_1+s_2+s_1s_2+s_{12}) | h_1 h_2 \rangle_A \\ & + \langle p_1 p_2 | (\epsilon_1 + \epsilon_2)s_{12} - s_{12}(\epsilon_1 + \epsilon_2) | h_1 h_2 \rangle_A + \langle p_1 p_2 | u_{12}^A + u_{12}^B | h_1 h_2 \rangle_A = 0, \end{aligned} \quad (22)$$

where

$$\langle h_1 | \epsilon_1 | h_2 \rangle \equiv \langle h_1 | t_1(1+s_1) + \tilde{u}_1 | h_2 \rangle, \quad (23)$$

$$\langle p_1 | \epsilon_1 | p_2 \rangle \equiv \langle p_1 | (1-s_1)t_1 + \tilde{u}_1 | p_2 \rangle, \quad (24)$$

$$\langle h_1 | \tilde{u}_1 | h_2 \rangle = \sum_{h'} \langle h_1 h' | v_{12}(1+s_1+s_2+s_1s_2+s_{12}) | h_2 h' \rangle_A, \quad (25)$$

$$\langle p_1 | \tilde{u}_1 | p_2 \rangle = \sum_{h'} \langle p_1 h' | (1-s_1)v_{12}(1+s_1+s_2) | p_2 h' \rangle_A - \sum_{p'} \langle p_1 p' | s_{12}v_{12} | p_2 p' \rangle_A, \quad (26)$$

$$\begin{aligned} \langle p | \tilde{u}_1 | h \rangle &= \langle p h' | t_2 s_{12} + (1-s_1)v_{12}(1+s_1+s_2+s_1s_2+s_{12}) | h h' \rangle_A \\ &+ \frac{1}{2} \sum_{h' h''} \sum_{p'} \{ 2 \langle h' h'' | v_{12} | p' h'' \rangle_A \langle p p' | s_{12} | h h' \rangle_A + \langle h' h'' | v_{12} | p' h \rangle_A \langle p p' | s_{12} | h' h'' \rangle_A \} \\ &+ \frac{1}{2} \sum_{h' h''} \frac{1}{2} \sum_{p' p''} 2 \langle h' h'' | v_{12} | p' p'' \rangle_A \{ 2 \langle p p' | s_{12} | h h' \rangle_A \langle p'' | s_1 | h'' \rangle + \langle p p' | s_{12} | h' h'' \rangle_A \langle p'' | s_1 | h \rangle \}, \end{aligned} \quad (27)$$

$$\begin{aligned} \langle p_1 p_2 | u_{12}^A | h_1 h_2 \rangle_A &\equiv \sum_{h' p'} \left[ \{ \langle p_2 h' | (1-s_1)v_{12} | p' h_1 \rangle_A + \sum_{p''} \langle p_2 h' | (1-s_1)v_{12} | p' p'' \rangle_A \langle p'' | s_1 | h_1 \rangle \} \langle p_1 p' | s_{12} | h_2 h' \rangle_A \right. \\ &\quad \left. - \{ \langle p_2 h' | (1-s_1)v_{12} | p' h_2 \rangle_A + \sum_{p''} \langle p_2 h' | (1-s_1)v_{12} | p' p'' \rangle_A \langle p'' | s_1 | h_2 \rangle \} \langle p_1 p' | s_{12} | h_1 h' \rangle_A \right] \end{aligned}$$

$$\begin{aligned}
& + \{ \langle p_1 h' | (1 - s_1) v_{12} | p' h_1 \rangle_A + \sum_{p''} \langle p_1 h' | (1 - s_1) v_{12} | p' p'' \rangle_A \langle p'' | s_1 | h_1 \rangle \} \langle p' p_2 | s_{12} | h_2 h' \rangle_A \\
& - \{ \langle p_1 h' | (1 - s_1) v_{12} | p' h_2 \rangle_A + \sum_{p''} \langle p_1 h' | (1 - s_1) v_{12} | p' p'' \rangle_A \langle p'' | s_1 | h_2 \rangle \} \langle p' p_2 | s_{12} | h_1 h' \rangle_A \Big], \quad (28)
\end{aligned}$$

$$\begin{aligned}
\langle p_1 p_2 | u_{12}^B | h_1 h_2 \rangle_A & \equiv 4 \frac{1}{2} \sum_{h' h''} \frac{1}{2} \sum_{p' p''} \langle h' h'' | v_{12} | p' p'' \rangle_A \{ \langle p_1 p' | s_{12} | h_1 h' \rangle_A \langle p_2 p'' | s_{12} | h_2 h'' \rangle_A \\
& - \langle p_1 p' | s_{12} | h_2 h' \rangle_A \langle p_2 p'' | s_{12} | h_1 h'' \rangle_A \}. \quad (29)
\end{aligned}$$

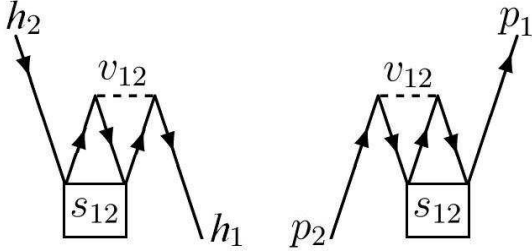


FIG. 2: Diagram representation of the  $s_{12}$  contribution to the one-body average potential  $\tilde{u}_1$ , Eqs. (25) and (26). The antisymmetrization is not shown explicitly.

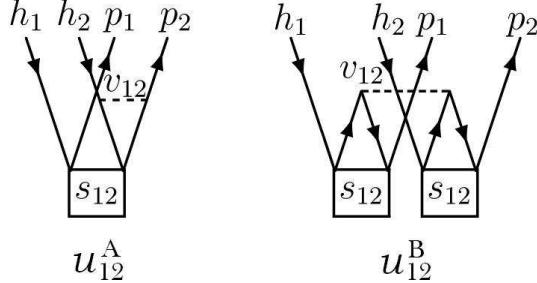


FIG. 3: Diagram representation of the  $s_{12}$  contribution to the two-body average potentials  $u_{12}^A$  and  $u_{12}^B$ , Eqs. (28) and (29), respectively. The antisymmetrization is not shown explicitly.

Note that  $\frac{1}{2} \sum_{hh'} |hh'\rangle_A \langle hh'|$  ( $\frac{1}{2} \sum_{pp'} |pp'\rangle_A \langle pp'|$ ) is a unit operator in an occupied (unoccupied) space. The  $s_{12}$  contribution to the single-particle potential  $\tilde{u}_1$ , Eqs. (25) and (26), is diagrammatically represented as in Fig. 2, and the potentials  $u_{12}^A$  and  $u_{12}^B$ , Eqs. (28) and (29), in Fig. 3. It can be checked that Eq. (21) completely agrees with the CCSD decoupling equation in the literature, as it should: e.g., Eq. (35) of ref. [6].

We need more explicit expressions to evaluate matrix elements such as  $\langle p_1 p_2 | (s_1 + s_2) v_{12} | h_1 h_2 \rangle_A$ , and algebraic calculations of the angular-momentum coupling for the numerical calculations of these expressions. We solve these non-linear equations for  $s_i$  and  $s_{ij}$  in an iterative way, using essentially the Newton method.

#### D. Energy and root-mean-square radius

The ground-state energy is obtained by Eq. (7). In the case that only two-body interactions are present, amplitudes higher than three-body  $s_{ijk}$  do not contribute to the CCM energy and the expression becomes:

$$\begin{aligned}
E_0 &= \sum_h \langle h | t_1 (1 + s_1) | h \rangle + \frac{1}{2} \sum_{hh'} \langle hh' | v_{12} \\
&\times (1 + s_1 + s_2 + s_1 s_2 + s_{12}) | hh' \rangle_A. \quad (30)
\end{aligned}$$

Effects of the higher order correlations enter through the one-body and two-body decoupling conditions. Although we do not consider contributions of a three-nucleon force in this article, it is instructive to present the energy expression in the presence of  $v_{ijk}$  and  $s_{ijk}$ , which is given in Appendix D. There we further rewrite the expression by introducing an effective two-nucleon interaction obtained from a three-nucleon interaction.

In the CCM framework, the evaluation of expectation values  $\langle \Psi | Q | \Psi \rangle$  of other observables  $Q$  than the energy needs explicit expansion of  $e^{S^\dagger} Q e^S$ . Although only linked-cluster diagrams are needed to be taken into account, a perturbative estimation in all-orders is not feasible. If the energy is determined variationally, we may use the Feynmann-Hellman theorem to obtain the matrix element of the given observable  $Q$  by solving the problem of the constrained Hamiltonian  $H + \lambda Q$ . That is, supposing the state  $|\Psi(\lambda)\rangle$  to be the solution of the forced Hamiltonian, the following relation holds.

$$\langle \Psi | Q | \Psi \rangle = \lim_{\lambda \rightarrow 0} \frac{d}{d\lambda} \langle \Psi(\lambda) | H + \lambda Q | \Psi(\lambda) \rangle. \quad (31)$$

Because the CCSD energy does not have a rigorous variational property,  $\langle \Psi(\lambda) | H | \Psi(\lambda) \rangle$  may depend linearly on  $\lambda$ , which introduces some uncertainty to the calculated expectation value of  $Q$ . Nevertheless, we calculate the root-mean-square (r.m.s.) radius of the  $^4\text{He}$  by this method, which is a square root of the expectation value of the operator

$$\begin{aligned}
Q_r &= \frac{1}{A} \sum_{i=1}^A (\mathbf{r}_i - \mathbf{R})^2 \\
&= \frac{1}{A} \left( 1 - \frac{1}{A} \right) \sum_{i=1}^A r_i^2 - \frac{2}{A^2} \sum_{i < j} \mathbf{r}_i \cdot \mathbf{r}_j, \quad (32)
\end{aligned}$$

where  $\mathbf{R} \equiv \frac{1}{A} \sum_i \mathbf{r}_i$  is the center-of-mass coordinate. Because the CCSD energy reaches almost variational limit in practice, the estimation by the constrained calculation is more reliable than the perturbative estimation in low-orders. As is shown explicitly in the next section, the reliability of the prescription of Eq. (31) is suggested by the fact that the calculated r.m.s. radii are almost independent on the oscillator constant of the harmonic oscillator basis.

It is helpful to note that the r.m.s. radius of the  $^4\text{He}$  reference state  $|\Phi_0\rangle \equiv |(0s)^4\rangle$  with the oscillator constant  $\nu$  is given by

$$\sqrt{\langle \Phi_0 | Q_r | \Phi_0 \rangle} = \frac{3}{2\sqrt{2\nu}}. \quad (33)$$

### III. RESULTS

We carry out numerical calculations in the harmonic oscillator basis. The oscillator constant is denoted by  $\nu$  which is related to the frequency  $\omega$  as  $\hbar\omega = \frac{\hbar^2}{m}\nu$  with  $m$  being the nucleon mass. The size of the harmonic oscillator basis is specified by the quantum number  $N_{max} = (2n + \ell)_{max}$ , where  $n$  is a nodal quantum number ( $n = 0, 1, 2, \dots$ ) and  $\ell$  an orbital angular momentum. The number of the major shells included is given by  $N_{max} + 1$ . To see the dependence of CCM calculations on the size of the model space, we use four different choices of  $N_{max}$ , as shown in Fig. 4.

As the first application of the reformulated CCM, we consider only  $^4\text{He}$ , for which the reference state  $|\Phi\rangle$  is taken to be  $(0s)^4$ . To keep the computational cost low, we set  $N_{max} \leq 22$  and introduce the cutoff at the upper right corner of the model space as in Fig. 4. Two-body partial waves up to  $J = 6$  are included. We employ two realistic nucleon-nucleon interactions; the CD-Bonn potential [20] and the AV18 potential [21]. The charge dependence of the CD-Bonn potential is averaged in actual calculations for the use of the isospin basis. These two potentials are different in their strength of the tensor force. The former is known to have relatively weak tensor components. Discussions are chiefly presented for the results of the CD-Bonn potential.

Two-body matrix elements of the bare nucleon-nucleon interaction in the harmonic oscillator basis are evaluated by the Talmi-Moshinsky transformation. Because the computation of Talmi-Moshinsky coefficients is time consuming when the oscillator quantum number becomes large, we use the approximation that the center-of mass (CM) quantum number is restricted to be  $(2n + \ell)_{CM} \leq 6$ . We have checked that the error due to this simplification is negligibly small.

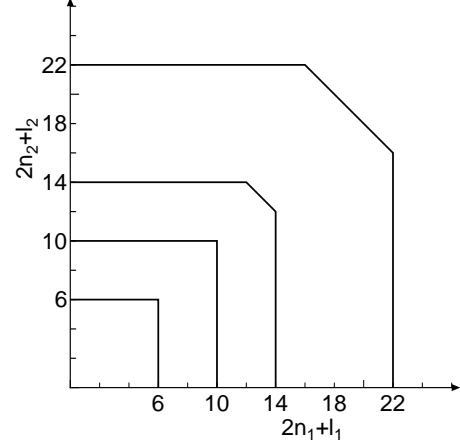


FIG. 4: Harmonic-oscillator model space for CCM. Four choices,  $(2n + \ell)_{max} = 6, 10, 14$ , and  $22$ , are used for numerical calculations.

#### A. Calculations with CD-Bonn bare interaction

Calculated CCSD ground-state energies of  $^4\text{He}$  with the CD-Bonn potential are shown in Fig. 5, as a function of the size of the harmonic-oscillator base,  $N \equiv 2n + \ell$ , with the oscillator constant  $\nu = 0.56 \text{ fm}^{-2}$ . As a reference, the energy of the Faddeev-Yakubovsky calculation [24] with the same interaction is also shown. Increasing the size of the model space, the CCSD energy goes down toward to the F-Y energy. However, at  $N_{max} = 22$ , the energy is still short by about 8 MeV to the reference value of the Faddeev-Yakubovsky calculation. When the AV18 potential is employed, the shortage is about 21 MeV, compared with the corresponding F-Y result of -24.3 MeV. This result is not surprising, because the s.p. space is not sufficient to properly treat the short-range correlation of the ordinary realistic nucleon-nucleon interaction. The momentum scale in the model space may be estimated by the expectation value of the square of the momentum operator  $\langle \mathbf{p}^2 \rangle = (N_{max} + \frac{3}{2})\nu$ . The number is  $\sqrt{\langle \mathbf{p}^2 \rangle} = 3.6 \text{ fm}^{-1}$  for  $N_{max} = 22$  and  $\nu = 0.56 \text{ fm}^{-2}$ , which is much smaller than the high momentum relevant to the nucleon-nucleon short-range correlation.

It is difficult in practice to employ a large harmonic oscillator basis for CCM calculations enough to deal with the nucleon-nucleon short-range correlation. The established wisdom in nuclear physics is to treat the short range singularity by solving the  $G$ -matrix equation as a two-body problem in the nuclear medium [25, 26]. Though the perturbative expansion in terms of  $G$ -matrices is a solid framework, the CCM provides a more systematic and compact way to treat higher-order correlations. One standard approximation besides the  $G$ -matrix approach is to use a two-step method, in which two-body correlations are initially treated in a large space and then solve many-body correlations in a restricted space. This strategy is adopted, e.g., in the unitary-

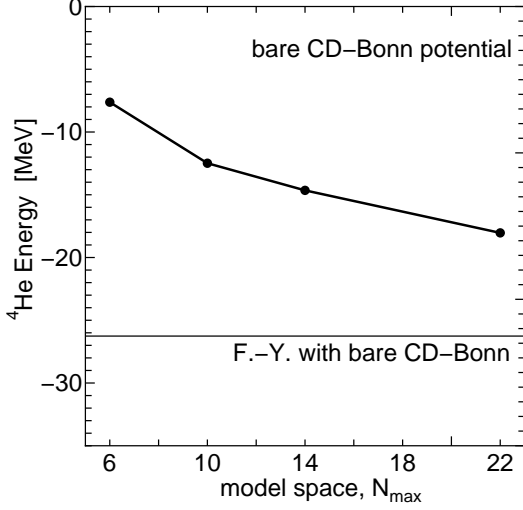


FIG. 5: Dependence of CCSD ground-state energies of  ${}^4\text{He}$  on the harmonic-oscillator model-space size  $N_{\max}$  with the bare CD-Bonn potential [20]. The oscillator constant is  $\nu = 0.56 \text{ fm}^{-2}$  ( $\hbar\omega = 23.2 \text{ MeV}$ ). The energy by the Faddeev-Yakubovsky calculation [24] is shown for reference.

model-operator approach [27].

A different method has been recently developed. Namely, the bare interaction is transformed to the half-on-shell two-body equivalent interaction in low-momentum space [3], which is free from the high-momentum singularity. This interaction has been shown to be used in perturbation calculations in a low-momentum space. Though the linkage between the harmonic oscillator basis and the low-momentum space is somewhat obscure and therefore the treatment in the harmonic oscillator basis from the beginning is desirable, we use the low-momentum space interaction in this paper because of its simplicity and possibilities of the comparison with calculations in the literature [14].

It is noted that in a restricted model space more than three-body correlations involving high-momentum states are totally dropped. These contributions are to be recovered by more than three-nucleon induced interactions in a restricted space. Otherwise some adjustable parameters may be introduced, if we take a viewpoint that high-momentum components of bare nucleon-nucleon interactions are themselves cannot be determined without uncertainties.

### B. Calculations with low-momentum interaction

In this subsection, calculated results for low-momentum space equivalent interactions of three cutoff momenta,  $\Lambda = 4.0, 3.0$ , and  $1.9 \text{ fm}^{-1}$ , are presented. The CCSD  ${}^4\text{He}$  ground-state energies and radii with the CD-Bonn potential are shown in Figs. 6 and 7 as a function of the size of the harmonic-oscillator basis.

Results with  $\Lambda = 1.9 \text{ fm}^{-1}$  show that the energy of

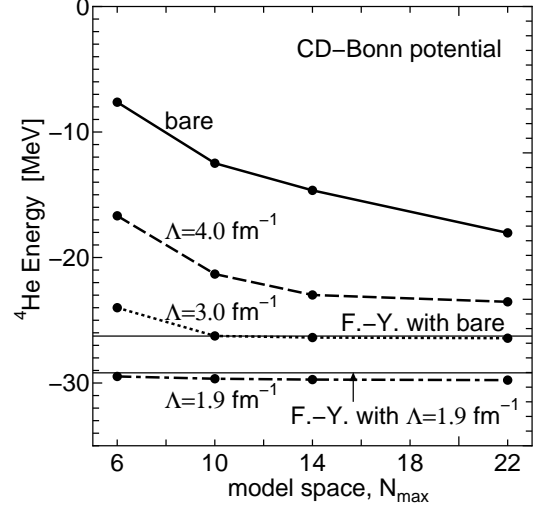


FIG. 6: Dependence of CCSD ground-state energies of  ${}^4\text{He}$  on the harmonic-oscillator model-space size  $(2n+\ell)_{\max}$  with low-momentum equivalent interactions of three cutoff momenta,  $\Lambda = 4.0, 3.0$ , and  $1.9 \text{ fm}^{-1}$ . The bare interaction is the CD-Bonn potential and the oscillator constant is  $\nu = 0.56 \text{ fm}^{-2}$  ( $\hbar\omega = 23.2 \text{ MeV}$ ).

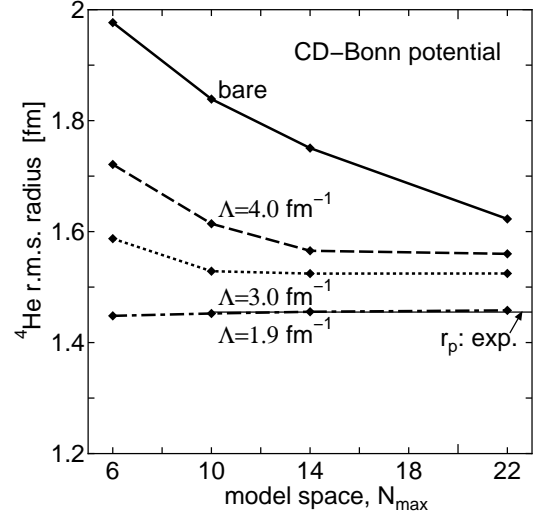


FIG. 7: Same as in Fig. 6, but for CCSD ground-state point-nucleon r.m.s. radii of  ${}^4\text{He}$ . The experimental point proton radius is shown as a guide, which is taken from ref. [28].

the Faddeev-Yakubovsky calculation with the same low-momentum equivalent interaction is almost reproduced already at  $N_{\max} = 6$ . This implies that if the two-body correlations are renormalized at  $\Lambda = 1.9 \text{ fm}^{-1}$ , more than three-body correlations in the model space scarcely change energy. The evaluated radius is also insensitive to the size of the model space for  $\Lambda = 1.9 \text{ fm}^{-1}$ . On the other hand, the difference between the energy with  $\Lambda = 1.9 \text{ fm}^{-1}$  and the F-Y energy with the bare interaction suggests that more than three-body correlations involving higher-momentum components are of the order

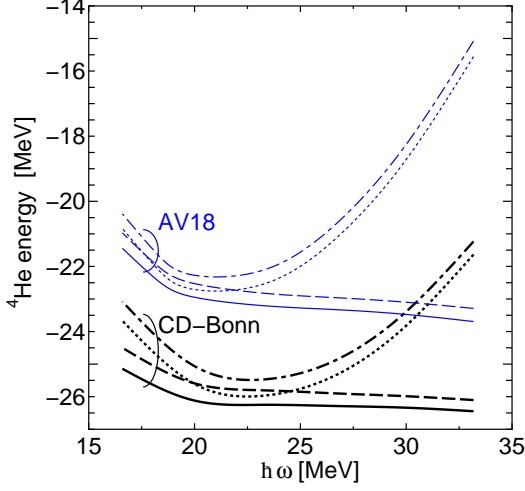


FIG. 8: Oscillator constant dependence of the ground-state energies of  ${}^4\text{He}$  for the model space  $N_{max} = 10$  with using the low-momentum equivalent interaction of  $\Lambda = 3 \text{ fm}^{-1}$ . The solid curve is the result of full CCSD calculation. The dashed curve shows the result with discarding  $u_{12}^A$  and  $u_{12}^B$ . The dotted and dot-dashed curves are results of the calculation for  $s_1 = 0$  with and without  $u_{12}^A$  and  $u_{12}^B$ , respectively.

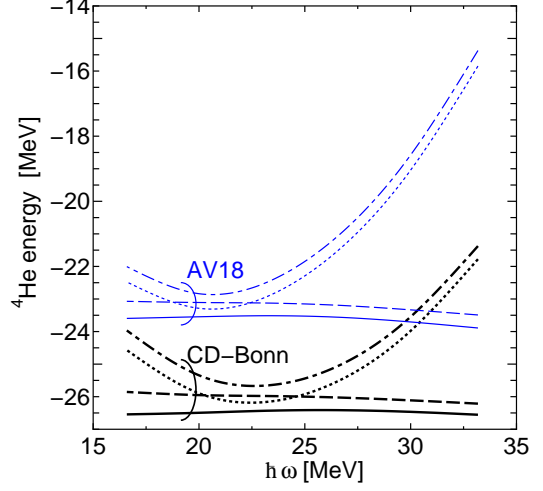


FIG. 10: Oscillator constant dependence of the ground-state energies of  ${}^4\text{He}$  for the model space  $N_{max} = 22$  with using the low-momentum equivalent interaction of  $\Lambda = 3 \text{ fm}^{-1}$ . The solid curve is the result of full CCSD calculation. The dashed curve shows the result with discarding  $u_{12}^A$  and  $u_{12}^B$ . The dotted and dot-dashed curves are results of the calculation for  $s_1 = 0$  with and without  $u_{12}^A$  and  $u_{12}^B$ , respectively.

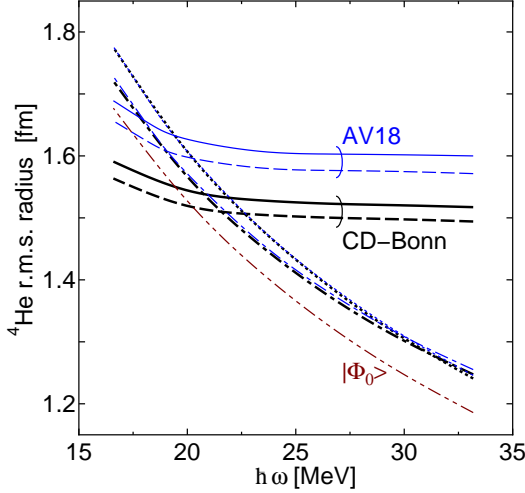


FIG. 9: Same as in Fig. 8, but for ground-state point-nucleon r.m.s. radii of  ${}^4\text{He}$ . The thin dot-dashed curve is almost indistinguishable from the bold dot-dashed curve. The r.m.s. radius of the reference state  $|\Phi_0\rangle$ , Eq. (33), is shown by a two-dot-dashed curve.

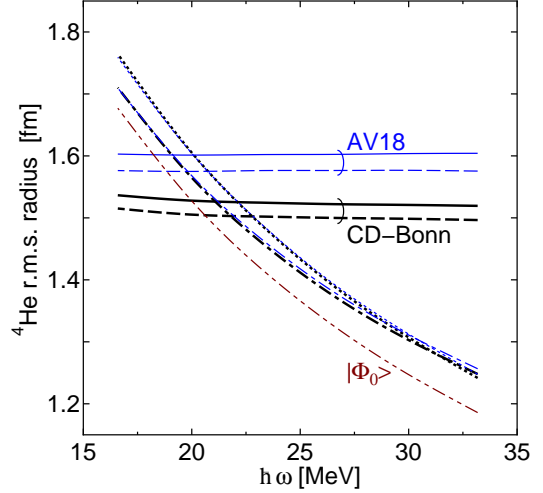


FIG. 11: Same as in Fig. 10, but for ground-state point-nucleon r.m.s. radii of  ${}^4\text{He}$ . The thin dot-dashed curve is almost indistinguishable from the bold dot-dashed curve. The r.m.s. radius of the reference state  $|\Phi_0\rangle$ , Eq. (33), is shown by a two-dot-dashed curve.

of a few MeV. Observing that the energy at  $\Lambda = 3 \text{ fm}^{-1}$  coincides with the F-Y energy, we see that the three-body correlations at the momentum range of  $2 \sim 3 \text{ MeV}/c$  is not negligible. It is remarked that the energy with  $\Lambda = 1.9 \text{ fm}^{-1}$  is slightly lower than the F-Y energy with the corresponding low-momentum interaction. This feature is different from the tendency in ref. [14].

Next, we turn to the oscillator constant dependence of the calculated results for CD-Bonn and AV18. This

case, we also show results of the calculation in which  $s_1$  is set to be 0 and/or the potentials  $u_{12}^{A,B}$  in Eq. (21) are omitted. Figs. 8 and 9 are the results for the model space  $N_{max} = 10$ , and Figs. 10 and 11 for  $N_{max} = 22$  with using the low-momentum equivalent interaction of  $\Lambda = 3 \text{ fm}^{-1}$ . Results from the CD-Bonn (AV18) potential are shown by thick (thin) curves.

The full CCSD results are seen to be almost independent on the oscillator constant both for ground-state



energies and radii of  $^4\text{He}$ , except for the region below  $\hbar\omega \simeq 20$  for  $N_{max} = 10$ . The tendency in the case of  $N_{max} = 10$  that the energy with larger  $\hbar\omega$  provides slightly lower energy is understandable, because the s.p. wave functions of the larger oscillator constant contain relatively larger high-momentum components. This point, however, needs to be clarified in detail together with the slight convex shape of the oscillator constant dependence of the energy. The difference of the solid and the long-dashed curves in Figs. 8~11 shows that the neglect of the potentials  $u_{12}^{A,B}$  does not much affect the energy and the radius. The ground-state energy becomes less attractive by about 0.5 MeV and the radius becomes slightly smaller by about 0.02 fm in the both cases of CD-Bonn and AV18.

The difference of the contributions of correlations described by  $u_{12}^{A,B}$  with CD-Bonn and AV18 reflects the different character of these interactions, typically observed in the strength of the tensor components. Together with the convergence with respect to the size of the model space, we see that the many-body problem with the low-momentum equivalent interaction is solved adequately by the CCM framework at the CCSD level.

If we neglect  $s_1$  terms from the beginning, the CCD approximation, calculated energies and radii vary with changing the oscillator constant of the model space, as Figs. 8~11 show. Increasing the frequency  $\hbar\omega$ , the energy attains a minimum value at  $\hbar\omega = 21 \sim 23$  MeV and the radius decreases monotonically in almost parallel with the r.m.s. radius of the reference state  $|\Phi_0\rangle$ , Eq. (33). Even in this case, the effect of  $u_{12}^{A,B}$  is comparable to the case of fully including  $s_1$ . It is interesting to observe that the difference between the energy with  $s_1 = 0$  at its minimum value and the full CCSD energy is rather small. The r.m.s. radii with and without  $s_1$  are also seen to coincide each other at the point where energies with and without  $s_1$  become close.

The order of 0.5 MeV of the difference between calculated energies with and without the  $u_{12}^{A,B}$  terms is smaller than that of the energy gain due to the two-body high-momentum correlations. This implies that the two-body correlations including high-momentum components are primarily important and the remaining many-body correlations summed up by  $u_{12}^{A,B}$  in a restricted model space plays a minor role in the magnitude of energy. This is consistent with the conventional understanding, regarding the justification of the independent particle picture in spite of the short-range repulsion of the bare nucleon-nucleon interaction.

The above observation suggests that three-body correlations including high-momentum components are worth to investigate quantitatively. On the other hand, in the renormalization-group view-point on which the development of low-momentum interaction [3] is conceptually based, such correlations should be hidden in adjustable parameters as far as low-energy properties of nuclei are concerned. When the experimental data at intermediate energy in nuclear physics is accumulated in the future,

these correlations will be addressed as the important subject to analyze.

#### IV. SUMMARY

We have evaluated the ground-state energy and radius of  $^4\text{He}$  in the reformulated coupled-cluster method in which many-body average potentials are introduced. This method was proposed by Suzuki in 1990's [19, 23], but has not been practiced for actual nuclei. The formulation clarifies the procedure to organize the Hamiltonian in a normal-ordered form with respect to the reference state, and thus the structure of the CCM approach as the many-body theory. The obtained decoupling equation in the truncation at the two-body correlation level, commonly referred to as the CCSD approximation, is arranged in a concise form as given in Eq. (22) by virtue of the average potential, although the content is necessarily not different from that of other CCM calculations [6].

Numerical calculations are carried out in the harmonic oscillator basis. Major shells up to  $N_{max} = 22$  are prepared, while the oscillator constant  $\nu$  is varied in the range of  $0.4 \sim 0.8 \text{ fm}^{-2}$ . Besides the bare CD-Bonn and AV18 nucleon-nucleon potentials, we show the results with using low-momentum equivalent interactions. The independence of the results on the oscillator constant  $\nu$  is demonstrated both for the ground-state energy and the radius. When we ignore the  $s_1$  transformation amplitude, the energy shows the parabolic dependence on  $\nu$  in the calculated range and the radius decreases monotonically with increasing  $\nu$ . It is interesting to see that the difference of the energies with and without  $s_1$  is minimized at around the point where the radii with and without  $s_1$  coincide.

It has been sometimes advocated [3] that different bare interactions collapse to universal low-momentum interaction. This property is well expected as far as the diagonal matrix elements are concerned, because on-shell matrix elements are directly related to experimental scattering data. However, the difference of inherent characters of each bare interaction which are typically characterized by the strength of tensor components persists in the low-momentum interaction.

There are several ways to extend the present stage of our calculations in the future. The estimation of the contributions beyond the  $s_1 + s_{12}$  approximation is necessary. The inclusion of  $s_{123}$ , however, affects the energy only through the change of  $s_1$  and  $s_{12}$ , when only two-body interactions are present. Therefore, the net effect of those higher correlations may be small. The estimation of the contribution of a three-nucleon interaction is important to quantitatively describe the saturation properties of nuclei. The expression for the contribution of the three-nucleon force to the ground-state energy is presented in Appendix D, which helps to understand the different character of the contributions of the three-nucleon force and three-body correlations (or an induced

three-nucleon force). As for the treatment of short-range singularity of the nucleon-nucleon interaction, it is desirable to renormalize the high-momentum component of the bare nucleon-nucleon interaction in a more seamless way, working always in a harmonic oscillator basis. Finally, numerical calculations should be extended to larger nuclei and also the consideration of excited states.

### Acknowledgments

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## Appendix A: Similarity transformation of the one-body operator

Remembering that the product of more than two transformation amplitudes in which the same suffix appears, e.g.  $s_1 s_{12}$ , vanishes, the similarity-transformation of the one-body operator  $\sum_i t_i$  leads to up to 4-body operators. The expansion of the similarity-transformation  $e^{-S} \sum_i t_i e^S$  with  $S = \sum_i s_i + \sum_{i<j} s_{ij} + \sum_{i<j<k} s_{ijk}$  provides the following terms:

$$\text{1-body part} \quad \sum_i (1 - s_i) t_i (1 + s_i), \quad (\text{A1})$$

$$\text{2-body part} \quad \sum_{i<j} \{ (t_i + t_j) s_{ij} - s_{ij} (t_i + t_j) - (s_i t_i + s_j t_j) s_{ij} - s_{ij} (t_i s_i + t_j s_j) \}, \quad (\text{A2})$$

$$\text{3-body part} \quad - \sum_{i,j,k(j \neq k)} \widehat{s_{ij} t_i s_{ik}} - \sum_{i,(j<k)} \{ s_i t_i \widehat{s_{ijk}} + \widehat{s_{ijk}} t_i s_i \}, \quad (\text{A3})$$

$$\text{4-body part} \quad - \sum_{i,j,(k<\ell)} (\widehat{s_{ik\ell} t_i s_{ij}} + \widehat{s_{ij} t_i s_{ik\ell}}), \quad (\text{A4})$$

where the widehat  $\widehat{ijk}$  in the suffix means that  $i, j$  and  $k$  are to be arranged in an ascending order.

## Appendix B: Similarity transformation of the two-body interaction

The expansion of the similarity-transformation  $e^{-S} \left( \sum_{i<j} v_{ij} \right) e^S$  provides up to 6-body operators. Explicit expressions are the following, omitting terms including  $s_{ijkl}$  and higher excitation operators. Note that the two-body part corresponds to  $\sum_{i<j} (\tilde{v}_{ij} - \tilde{u}_{ij})$  in Eq. (11), the three-body part to  $\sum_{i<j<k} (\tilde{v}_{ijk} - \tilde{u}_{ijk})$  originating from the two-body interaction  $v_{ij}$ , and so on.

$$\text{2-body part} \quad \sum_{i<j} (1 - s_i - s_j + s_i s_j - s_{ij}) v_{ij} (1 + s_i + s_j + s_i s_j + s_{ij}), \quad (\text{B1})$$

$$\begin{aligned} \text{3-body part} \quad & \sum_{i<j} \sum_k \{ (1 - s_i - s_j + s_i s_j - s_{ij}) v_{ij} (\widehat{s_{ik}} + \widehat{s_{jk}} + \widehat{s_{ik}} s_j + \widehat{s_{jk}} s_i + \widehat{s_{ijk}}) \\ & - (\widehat{s_{ik}} + \widehat{s_{jk}} - \widehat{s_{ik}} s_j - \widehat{s_{jk}} s_i + \widehat{s_{ijk}}) v_{ij} (1 + s_i + s_j + s_i s_j + s_{ij}) \}, \end{aligned} \quad (\text{B2})$$

$$\begin{aligned} \text{4-body part} \quad & \sum_{i<j} \sum_{k<\ell} \{ (1 - s_i - s_j - s_{ij} + s_i s_j) v_{ij} (\widehat{s_{ik\ell}} + \widehat{s_{j\ell}} + \widehat{s_i s_{j\ell}} + \widehat{s_j s_{ik\ell}}) \\ & - (\widehat{s_{ik\ell}} + \widehat{s_{j\ell}} - \widehat{s_i s_{j\ell}} - \widehat{s_j s_{ik\ell}}) v_{ij} (1 + s_i + s_j + s_{ij} + s_i s_j) \} \\ & + \sum_{i<j} \sum_{k \neq \ell} \{ (1 - s_i - s_j - s_{ij} + s_i s_j) v_{ij} \widehat{s_{ik}} \widehat{s_{j\ell}} + \widehat{s_{ik}} \widehat{s_{j\ell}} v_{ij} (1 + s_i + s_j + s_{ij} + s_i s_j) \\ & - (\widehat{s_{ik}} + \widehat{s_{j\ell}} + \widehat{s_{ijk}} - \widehat{s_i s_{jk}} - \widehat{s_j s_{ik}}) v_{ij} (\widehat{s_{i\ell}} + \widehat{s_{j\ell}} + \widehat{s_{ij\ell}} + \widehat{s_i s_{j\ell}} + \widehat{s_j s_{i\ell}}) \}, \end{aligned} \quad (\text{B3})$$

$$\begin{aligned} \text{5-body part} \quad & \sum_{i<j} \sum_{k<\ell} \sum_m \{ (1 - s_i - s_j - s_{ij} + s_i s_j) v_{ij} (\widehat{s_{ik\ell}} \widehat{s_{jm}} + \widehat{s_{j\ell}} \widehat{s_{im}}) \\ & + (\widehat{s_{ik\ell}} \widehat{s_{jm}} + \widehat{s_{j\ell}} \widehat{s_{im}}) v_{ij} (1 + s_i + s_j + s_{ij} + s_i s_j) \\ & - (\widehat{s_{im}} + \widehat{s_{jm}} + \widehat{s_{ijm}} - \widehat{s_i s_{jm}} - \widehat{s_j s_{im}}) v_{ij} (\widehat{s_{ik\ell}} + \widehat{s_{j\ell}} + \widehat{s_i s_{j\ell}} + \widehat{s_j s_{ik\ell}}) \} \end{aligned}$$

$$\begin{aligned}
& -(s_{ik\ell} + s_{jk\ell} - s_i s_{jkl} - s_j s_{ikl}) v_{ij} (s_{im} + s_{jm} + s_{ijm} + s_i s_{jm} + s_j s_{im}) \\
& + \sum_{i < j} \sum_{k \neq \ell \neq m} \{ -(s_{ik} + s_{jk} + s_{ijk} - s_i s_{jk} - s_j s_{ik}) v_{ij} s_{il} s_{jm} \\
& + s_{il} s_{jm} v_{ij} (s_{ik} + s_{jk} + s_{ijk} - s_i s_{jk} - s_j s_{ik}) \}, \tag{B4}
\end{aligned}$$

$$\begin{aligned}
\text{6-body part } & \sum_{i < j} \sum_{k < \ell} \sum_{m < n} \{ (1 - s_i - s_j - s_{ij} + s_i s_j) v_{ij} s_{ik\ell} s_{jmn} + s_{ik\ell} s_{jmn} v_{ij} (1 + s_i + s_j + s_{ij} + s_i s_j) \\
& - (s_{ik\ell} + s_{jk\ell} - s_i s_{jkl} - s_j s_{ikl}) v_{ij} (s_{imn} + s_{jmn} + s_i s_{jmn} + s_j s_{imn}) \} \\
& + \sum_{i < j} \sum_{k, \ell} \sum_{m < n} \{ (s_{il} s_{jmn} + s_{jl} s_{imn}) v_{ij} (s_{ik} + s_{jk} + s_{ijk} + s_i s_{jk} + s_j s_{ik}) \\
& - (s_{ik} + s_{jk} + s_{ijk} - s_i s_{jk} - s_j s_{ik}) v_{ij} (s_{il} s_{jmn} + s_{jl} s_{imn}) \\
& + s_{ik} s_{jl} v_{ij} (s_{imn} + s_{jmn} + s_i s_{jmn} + s_j s_{imn}) - (s_{imn} + s_{jmn} - s_i s_{jmn} - s_j s_{imn}) v_{ij} s_{ik} s_{jl} \} \\
& + \sum_{i < j} \sum_{k \neq \ell \neq m \neq n} s_{ik} s_{jl} v_{ij} s_{im} s_{jn}. \tag{B5}
\end{aligned}$$

### Appendix C: Similarity transformation of three-nucleon interaction

A three-body interaction  $v_{ijk}$  give the following three-body terms in the similarity-transformation. More than 4-body operators are not shown for the sake of simplicity.

$$\begin{aligned}
& \sum_{i < j < k} (1 - s_i - s_j - s_k - s_{ij} - s_{jk} - s_{ik} + s_i s_j + s_i s_k + s_j s_k - s_{ijk} + s_i s_{jk} + s_j s_{ik} + s_k s_{ij} - s_i s_j s_k + s_{ijk}) \\
& \times v_{ijk} (1 + s_i + s_j + s_k + s_{ij} + s_{jk} + s_{ik} + s_i s_j + s_i s_k + s_j s_k + s_{ijk} + s_i s_{jk} + s_j s_{ik} + s_k s_{ij} + s_i s_j s_k + s_{ijk}). \tag{C1}
\end{aligned}$$

### Appendix D: Expression of total energy with three-nucleon interaction

When the Hamiltonian contains a three-nucleon interaction,  $\sum_{i < j < k} v_{ijk}$ , the energy obtained from Eq. (7) becomes

$$\begin{aligned}
E_0 = & \sum_h \langle h | t_1 (1 + s_1) | h \rangle + \frac{1}{2} \sum_{hh'} \left\{ \langle hh' | v_{12} | hh' \rangle_A + \sum_p 2 \times \langle hh' | v_{12} | ph' \rangle_A \langle p | s_1 | h \rangle \right. \\
& + \frac{1}{2} \sum_{pp'} 2 \times \langle hh' | v_{12} | pp' \rangle_A \langle p | s_1 | h \rangle \langle p' | s_1 | h' \rangle + \frac{1}{2} \sum_{pp'} \langle hh' | v_{12} | pp' \rangle_A \langle pp' | s_{12} | hh' \rangle \} \\
& + \frac{1}{6} \sum_{hh'h''} \{ \langle hh'h'' | v_{123} (1 + s_{123}) | hh'h'' \rangle_A + 3 \sum_p \langle hh'h'' | v_{123} | ph'h'' \rangle_A \langle p | s_1 | h \rangle \\
& + \frac{1}{2} \sum_{pp'} 6 \times \langle hh'h'' | v_{123} | pp'h'' \rangle_A \langle p | s_1 | h \rangle \langle p' | s_1 | h' \rangle + \frac{1}{2} \sum_{pp'} 3 \times \langle hh'h'' | v_{123} | pp'h'' \rangle_A \langle pp' | s_{12} | hh' \rangle_A \\
& + \frac{1}{6} \sum_{pp'p''} 9 \times \langle hh'h'' | v_{123} | pp'p'' \rangle_A \langle pp' | s_{12} | hh' \rangle_A \langle p'' | s_1 | h'' \rangle \}. \tag{D1}
\end{aligned}$$

It is useful to introduce the two-body interaction  $v_{12(3)}$  by holding the one coordinate of  $v_{123}$  with occupied states,

$$\langle a_1 a_2 | v_{12(3)} | a_3 a_4 \rangle_A \equiv \sum_h \langle a_1 a_2 h | v_{123} | a_3 a_4 h \rangle_A. \tag{D2}$$

Using this notation, the energy  $E_0$  is written in a concise form as

$$E_0 = \sum_h \langle h | t_1 (1 + s_1) | h \rangle + \frac{1}{2} \sum_{hh'} \left\{ \langle hh' | v_{12} + \frac{1}{3} v_{12(3)} | hh' \rangle_A + \sum_p 2 \times \langle hh' | v_{12} + \frac{1}{2} v_{12(3)} | ph' \rangle_A \langle p | s_1 | h \rangle \right.$$

$$\begin{aligned}
& + \frac{1}{2} \sum_{pp'} 2 \times \langle hh' | v_{12} + v_{12(3)} | pp' \rangle_A \langle p | s_1 | h \rangle \langle p' | s_1 | h' \rangle + \frac{1}{2} \sum_{pp'} \langle hh' | v_{12} + v_{12(3)} | pp' \rangle_A \langle pp' | s_{12} | hh' \rangle_A \Bigg\} \\
& + \frac{1}{6} \sum_{hh'h''} \left\{ \langle hh'h'' | v_{123} s_{123} | hh'h'' \rangle_A + \frac{1}{6} \sum_{pp'p''} 9 \times \langle hh'h'' | v_{123} | pp'p'' \rangle_A \langle pp' | s_{12} | hh' \rangle_A \langle p'' | s_1 | h'' \rangle \right\}. \quad (D3)
\end{aligned}$$

The factors  $\frac{1}{3}$  and  $\frac{1}{2}$  in front of  $v_{12(3)}$  in the second and third terms come from the statistical weight and are naturally derived. The necessity of these factors are recently pointed out by Hebeler and Schwenk in Ref. [29]. It is noted, however, we also have to consistently include  $v_{ijk}$  and  $s_{ijk}$  in decoupling equations. The expressions become complicated, which are beyond the scope of this article.

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